

Concurrent materials design

Gareth Conduit

Patents GB1302743.8 (2013), EP14153898.3 (2014), US 2014/177578 (2014)

Patents GB1307533.8 (2013), EP14161255.6 (2014), US 2014/223465 (2014)

Patent GB1307535.3 (2013)

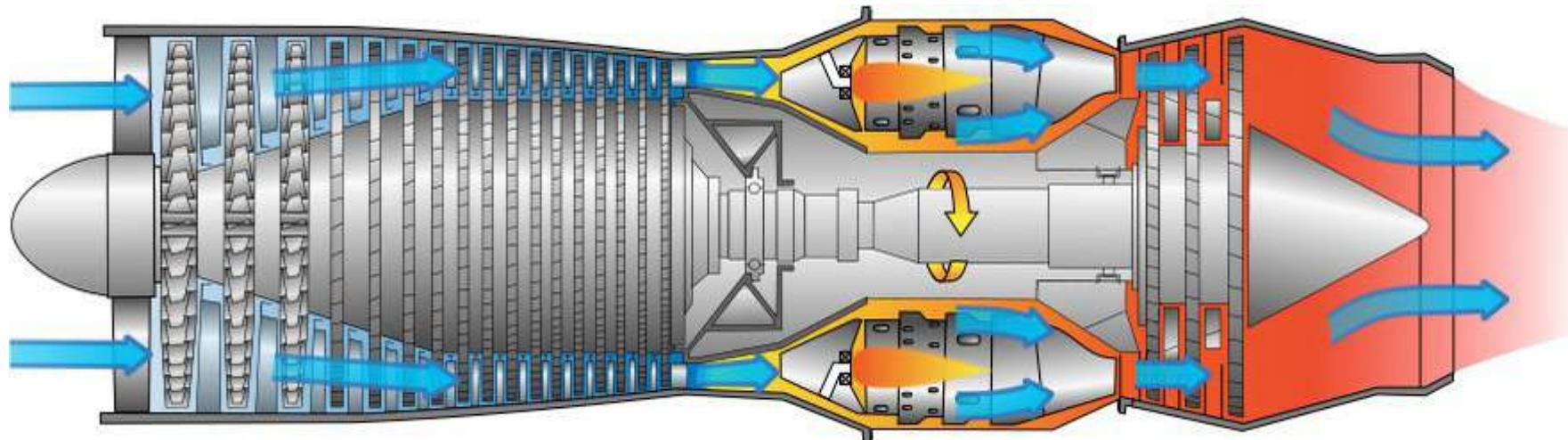
Patent US 2013/0052077 A1 (2013)

Acta Materialia, **61**, 3378 (2013)

Intermetallics, **48**, 62 (2014)

Theory of Condensed Matter Group, Department of Physics

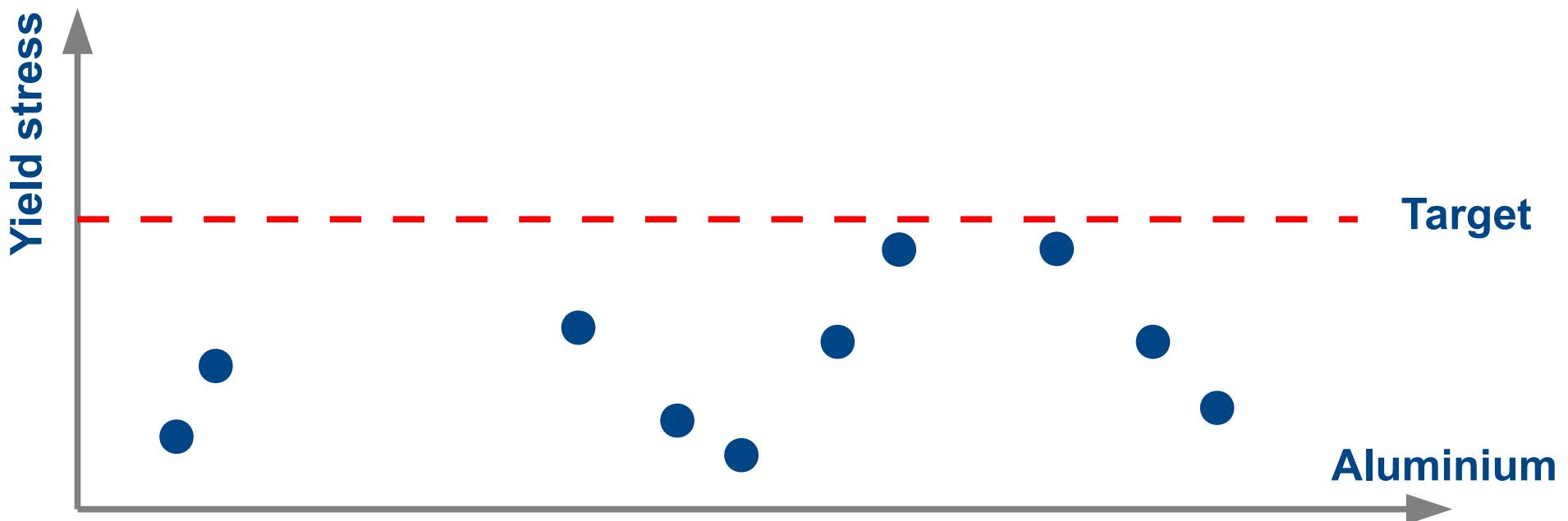
Jet engine: turbine discs



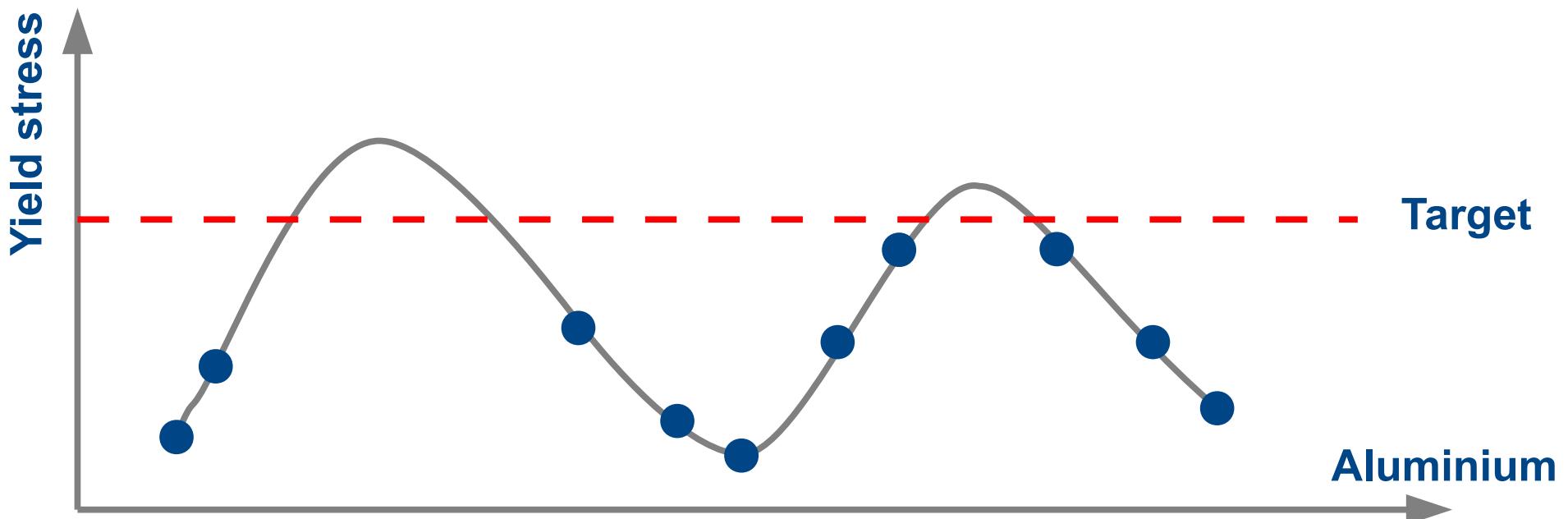
Designing a new alloy – what is required?



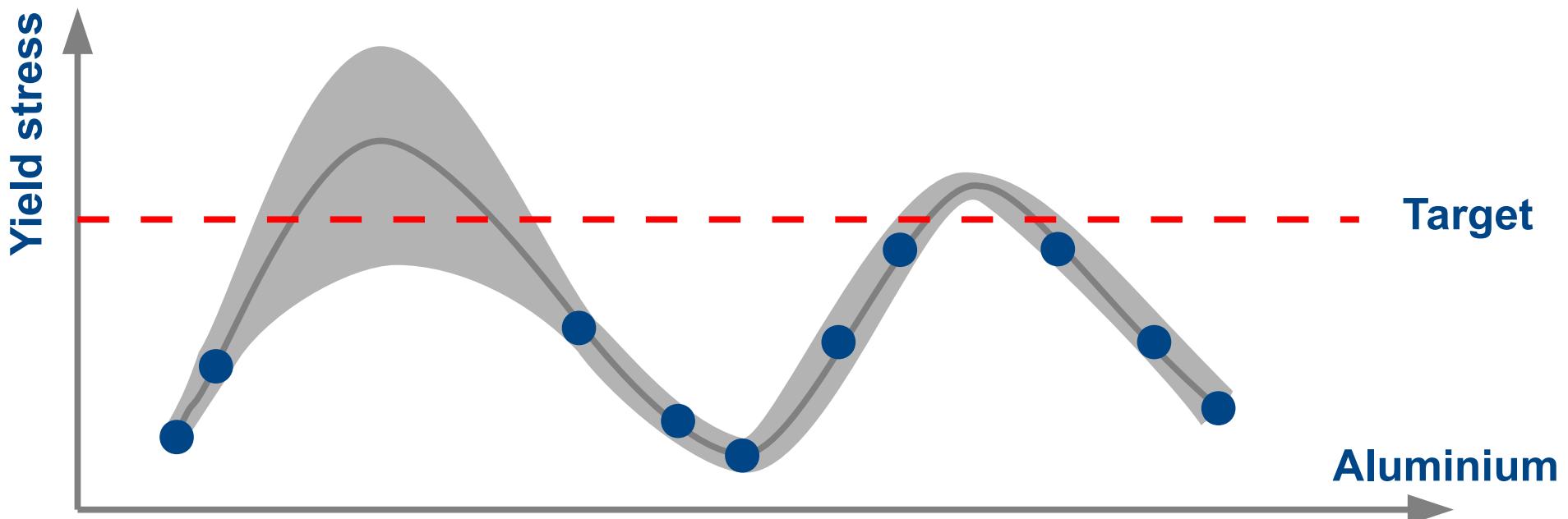
Neural network fitting & optimization



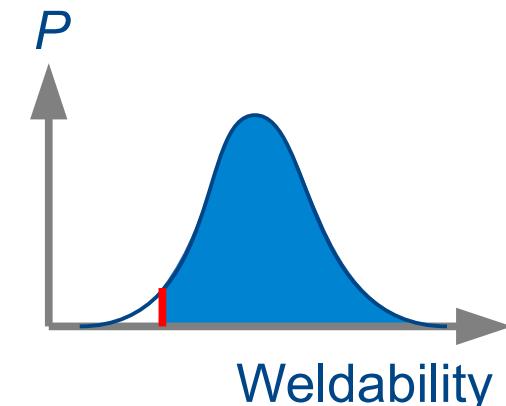
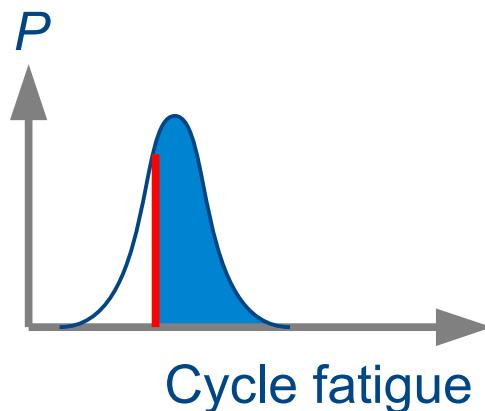
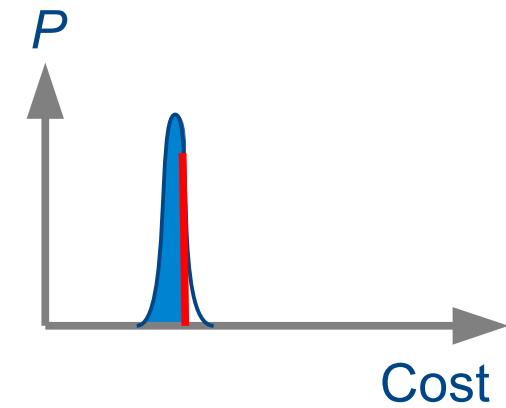
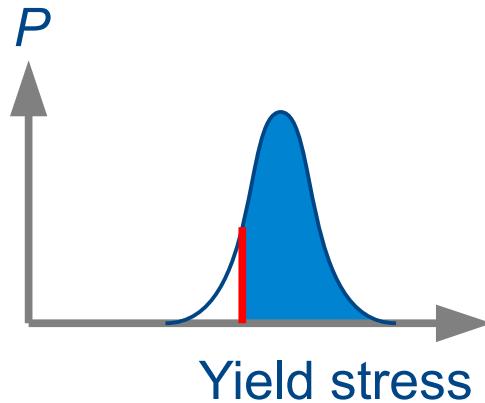
Neural network fitting & optimization



Neural network fitting & optimization



Probability



Probability of
alloy satisfying
all properties

Ni-base superalloy

Cost

32.1 \$lb⁻¹

Density

8240 kgm⁻³

Precipitate content

48 %

Phase stability

99.5 %

Solvus temperature

1080 C

Yield stress

1070 MPa

Ultimate tensile strength

1438 MPa

300hr stress rupture

980 MPa

Cr activity (oxidation resis.)

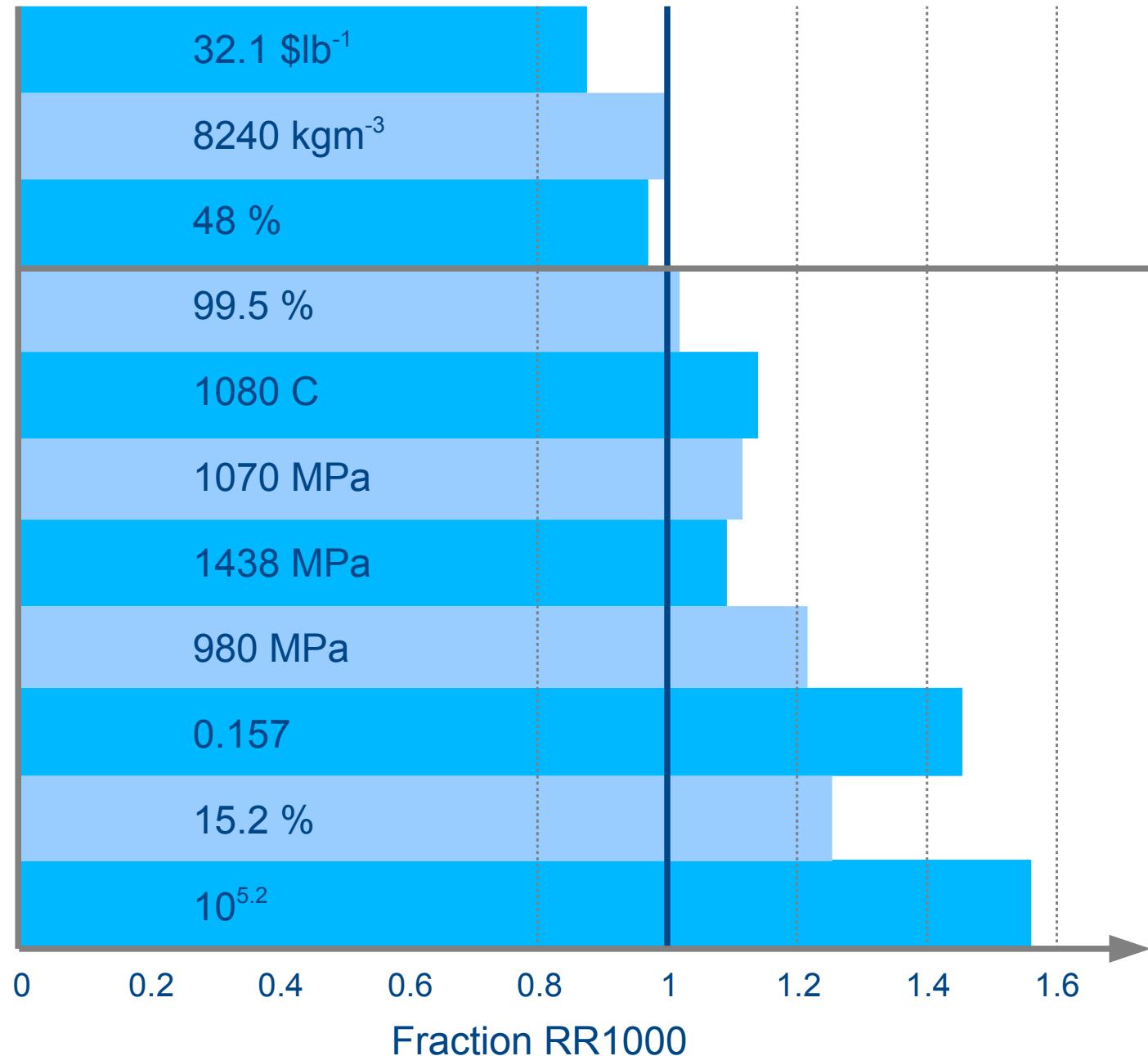
0.157

Tensile elongation

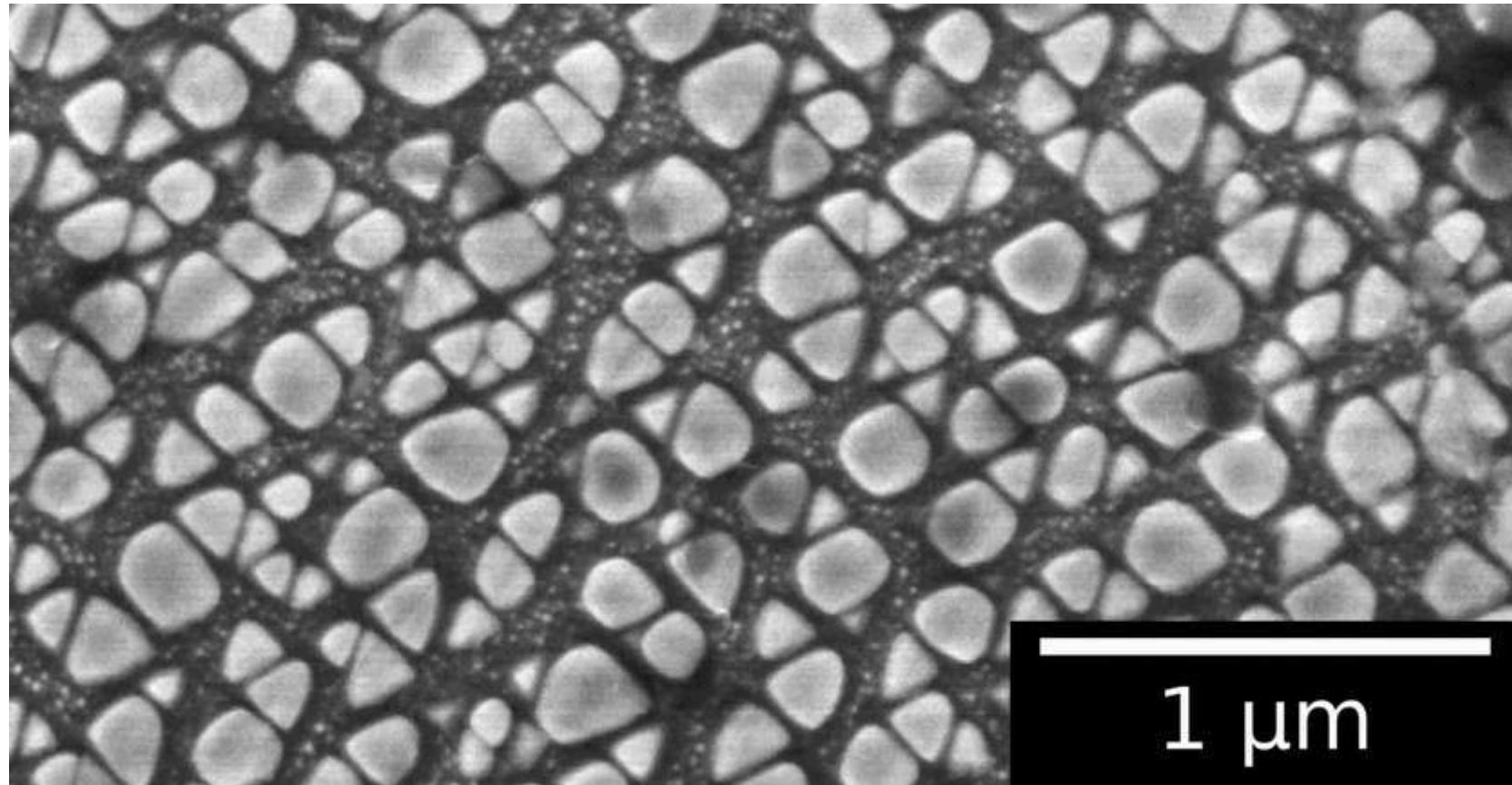
15.2 %

Fatigue life

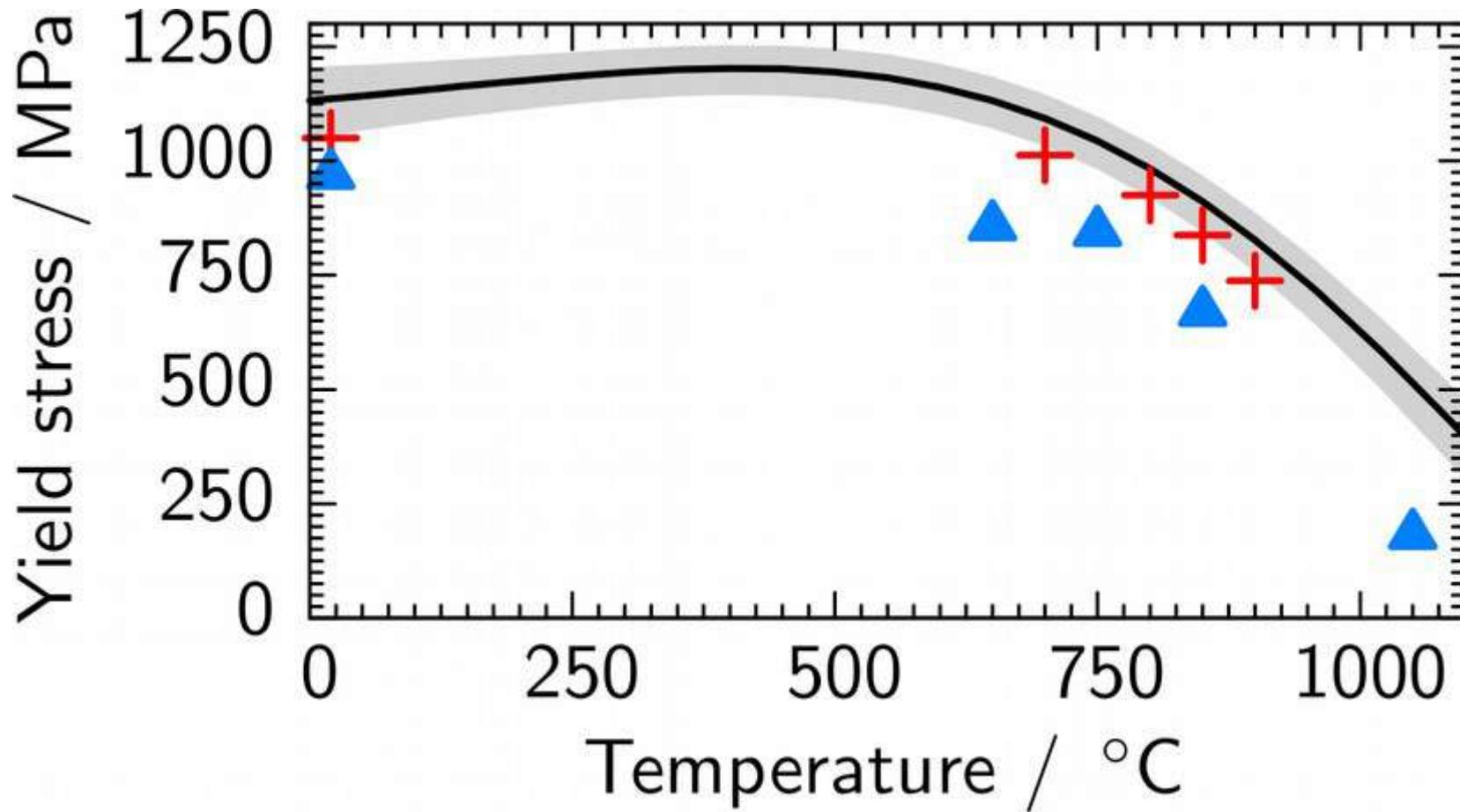
10^{5.2}



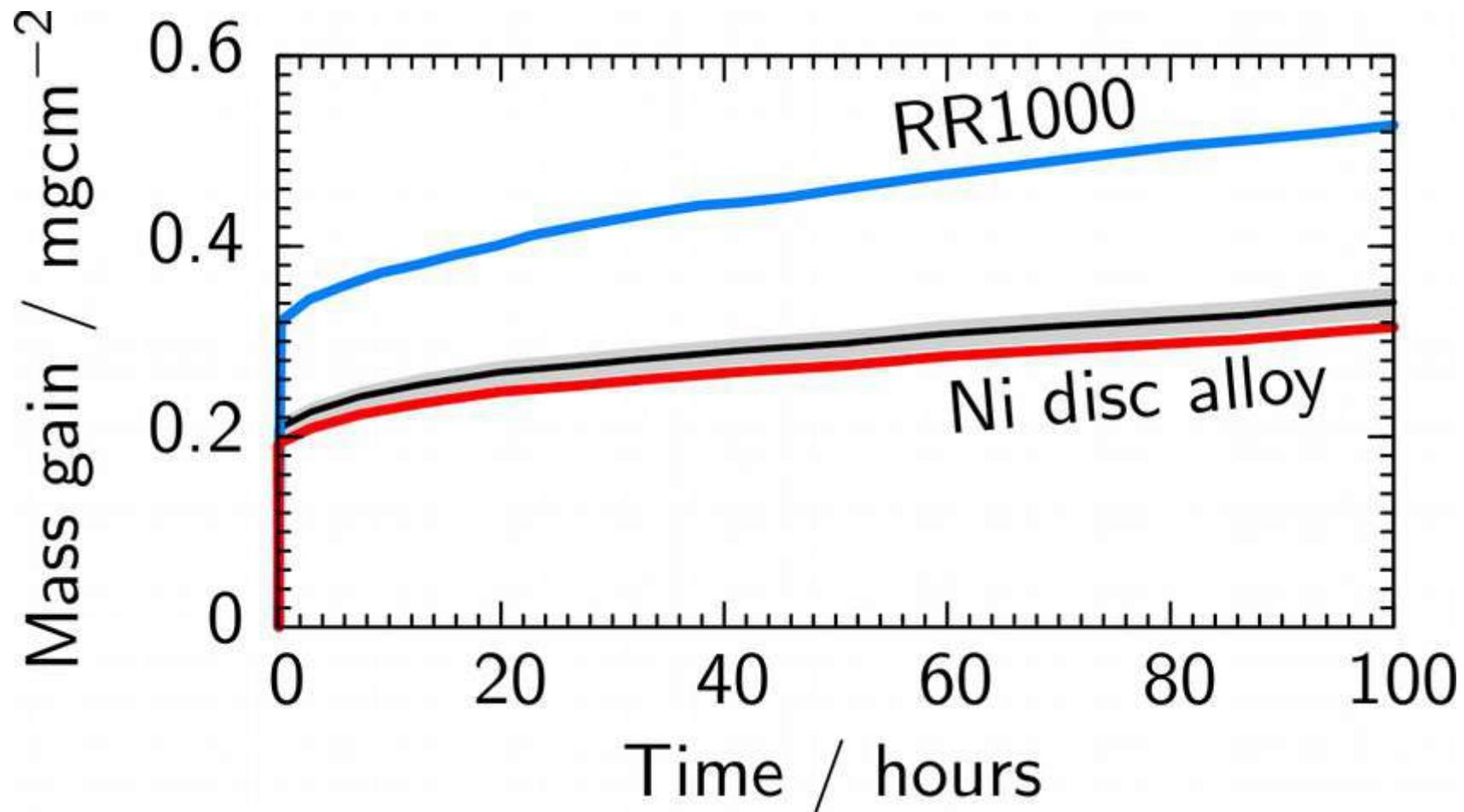
Ni-base superalloy



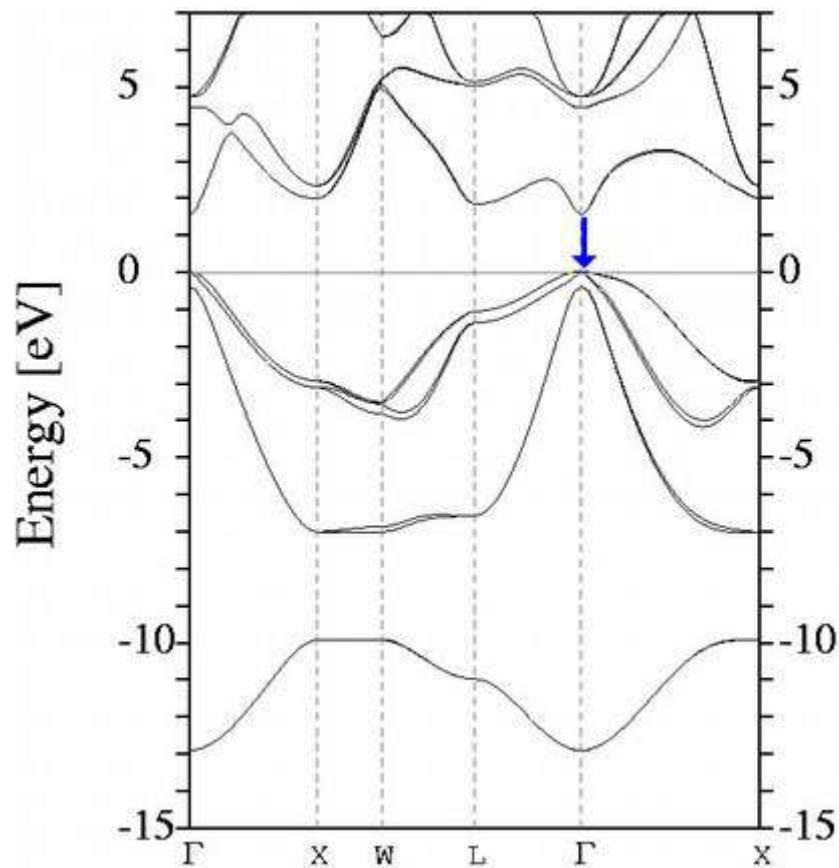
Ni-base superalloy



Ni-base superalloy



Semiconductors

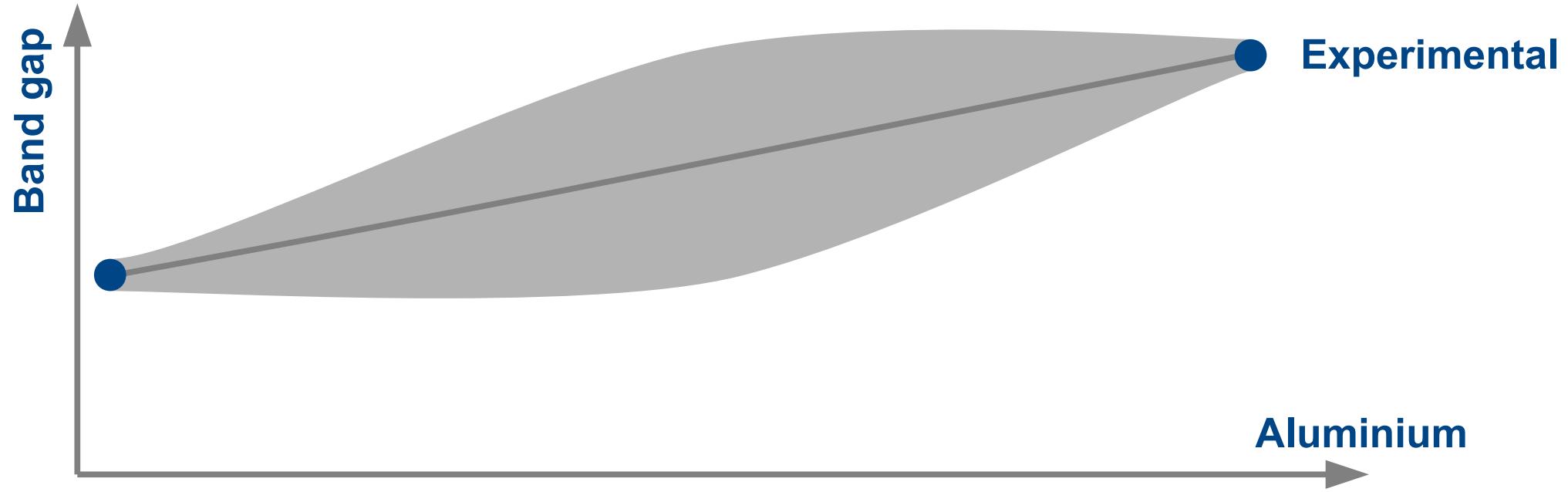


100 points for band gap, efficacy

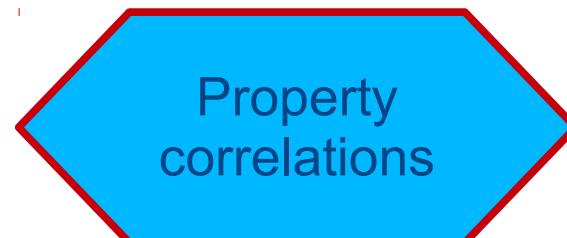
Property correlations

Band structure: band gap, density of states, effective mass

Semiconductors

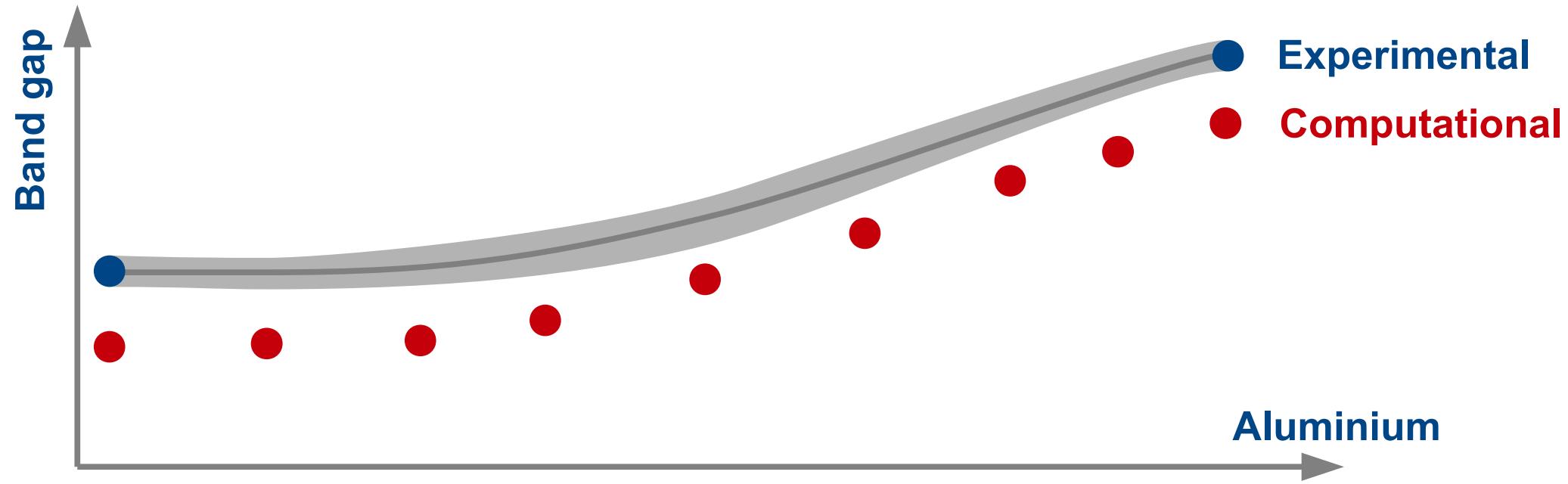


100 points for band gap, efficacy



Band structure: band gap, density of states, effective mass

Semiconductors



100 points for band gap, efficacy

Property correlations

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Prospects in the future

Take advantage of experimental databases to develop Ni and Mo-based alloys

Combine further first principles approaches to build new databases and guide extrapolation

Projects with Rolls Royce, Samsung, Royal Society Brian Mercer Feasibility award

Long-term goal of concurrent materials design